NUMERICAL SIMULATION OF THE COMBUSTION OF FUEL DROPLETS: AN AEROSPACE TECHNOLOGY OVERVIEW

Presented by:

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Numerical Simulation of the Combustion of Fuel Droplets; Finite Rate Kinetics and Flame Zone Grid Adaptation (CEFD)
A NASA Nebraska Space Grant and EPSCoR Sponsored Research Endeavor

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Running head: Combustion of Fuel Droplets

Numerical Simulation of the Combustion of Fuel Droplets;

Finite Rate Kinetics and Flame Zone Grid Adaptation (CEFD)

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Abstract

The NASA Nebraska Space Grant (NSGC) & EPSCoR programs have continued their effort to support outstanding research endeavors by funding the Numerical Simulation of the Combustion of Fuel Droplets study at the University of Nebraska at Lincoln (UNL). This team of researchers has developed a transient numerical model to study the combustion of suspended and moving droplets. The engines that propel missiles, jets, and many other devices are dependent upon combustion. Therefore, data concerning the combustion of fuel droplets is of immediate relevance to aviation and aeronautical personnel, especially those involved in flight operations. The experiments being conducted by Dr. Gogos' and Dr. Nayagam's research teams, allow investigators to gather data for comparison with theoretical predictions of burning rates, flame structures, and extinction conditions. "The consequent improved fundamental understanding of droplet combustion may contribute to the clean and safe utilization of fossil fuels" (Williams, Dryer, Haggard & Nayagam, 1997, ¶ 2). The present state of knowledge on convective extinction of fuel droplets derives from experiments conducted under normal gravity conditions. However, any data obtained with suspended droplets under normal gravity are grossly affected by gravity. The need to obtain experimental data under microgravity conditions is therefore well justified and addresses one of the goals of NASA's Human Exploration and Development of Space (HEDS) microgravity combustion experiment.

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Rationale

"The engines that propel missiles, jets, and many other devices are dependent upon combustion. Liquid fuel is sprayed into an engine chamber where it evaporates and burns, generating the thrust that propels the object forward" (Mashavek, 2001, ¶ 1). The amount of thrust created depends on many factors, including pressure, temperature, the fuel droplet evaporation rate, and turbulence. Therefore, data concerning the combustion of fuel droplets is of immediate relevance to aviation and aeronautical personnel, especially those involved in flight operations.

"The combustion of fuel droplets is an important part of many operations, such as the heating of furnaces for materials processing or home heating, power production by gas turbines, and combustion of gasoline in a car's engine" (Williams, Dryer, Haggard & Nayagam, 1997, ¶ 2). The Earth's gravity prevents many theoretical predictions involving fuel droplet combustion. Additionally, drop towers and aircraft are unsuitable for this type of experimentation due to time constraints and unacceptable levels of microgravity. The experiments being conducted by Dr. Gogos' and Dr. Nayagam's research teams, allow investigators to gather data for comparison with theoretical predictions of burning rates, flame structures, and extinction conditions. "The consequent improved fundamental understanding of droplet combustion may contribute to the clean and safe utilization of fossil fuels" (Williams, Dryer, Haggard & Nayagam, 1997, ¶ 2).

The present state of knowledge on convective extinction of fuel droplets derives from experiments conducted under normal gravity conditions. "Due to the increase in the extinction

velocity with droplet diameter, under extinction conditions natural convection becomes

negligible at large 'droplet' (porous sphere) diameters and important at smaller droplet

diameters" (Bowen, Woods, Narayanan, Smith, & Gogos, 2000, 4.3.3 p. 1). As a result, any data

obtained with suspended droplets under normal gravity are grossly affected by gravity. The need

to obtain experimental data under microgravity conditions is therefore well justified and

addresses one of the goals of NASA's Human Exploration and Development of Space (HEDS)

microgravity combustion experiment.

NSGC & EPSCoR Background and Research Involvement

The Nebraska Space Grant Consortium at the University of Nebraska at Omaha develops

research infrastructure and enhances the quality of aerospace research and education throughout

the state. This grant provides national leadership in applied aspects of aeronautics and allows

Nebraska colleges and universities to implement a balanced program of research, education, and

public service programs related to aeronautics, space science, and technology. The grant

administers funds to recruit and train professionals for careers in the aerospace industry.

EPSCoR (Experimental Program to Stimulate Competitive Research) assists states with

low levels of federal research and development support, thus responding to a Congressional

concern about increasing the geographic base of federal research support. Nebraska EPSCoR is

a statewide effort, which provides leadership for development of research and development in

science and engineering throughout the state. Specific to the University of Nebraska at Omaha is

the Aeronautics Education, Research, and Industry Alliance (AERIAL), a comprehensive, multi-

faceted, 5 year NASA EPSCoR 2000 initiative. This contributes substantially to the strategic

research and technology priorities of NASA while intensifying Nebraska's rapidly growing

aeronautics research and development endeavors.

The partnership between the NASA Nebraska Space Grant (NSGC) & EPSCoR programs allows for the selection of outstanding research projects that positively impact aeronautical technology advancement. These programs have continued their effort to support such research endeavors by funding the Numerical Simulation of the Combustion of Fuel Droplets study at the University of Nebraska at Lincoln (UNL).

The CEFD Concept

Dr. Vehda Nayagam guides the Microgravity Combustion Science Program in San Diego, CA. This program is conducting a project flight definition experiment to obtain data under microgravity conditions. The UNO CEFD collaborative research team (CRT) is developing a new comprehensive numerical model for the convective extinction of fuel droplets to validate this model. The data collected from each institution contributes to one of the long-term goals of the HEDS microgravity combustion program. Specifically, that which promotes "understanding that will permit lessons learned in microgravity combustion experiments and modeling to be used in optimizing combustion devices here on Earth."

A team of researchers from the University of Nebraska – Lincoln, led by Dr. George Gogos, is conducting a comprehensive computational study of fuel droplet combustion at atmospheric pressure and zero-gravity ambient conditions under forced convection. Through a collaborative effort with NASA Glenn Research Center, Dr. Gogos and his colleagues are developing a science education component that demonstrates how the combustion process changes due to microgravity.

Simplified as well as detailed chemical kinetics are employed in the research. The studies provide insights that can be applied to improve liquid fuel combustion with greater efficiency and safety, and reduce environmentally-adverse effects. In view of the detailed

chemical kinetics, substantial complexities and uncertainties are involved in modeling combustion of a moving droplet through the currently finding experimental research on combustion of a moving droplet through the Microgravity Combustion Science Program.

The research focuses on the validated modeling of two key topics: a) Transient combustion of a moving droplet with simplified chemical kinetics; and b) Transient combustion of a moving droplet with detailed chemical kinetics. The first topic is currently being addressed, whereas the second one is a longer-term research project. This work is a direct extension of research funded by the NASA Nebraska Space Grant and EPSCoR Programs. "Dr. Gogos' studies on droplet combustion at atmospheric pressure include combustion of moving droplets with infinitely fast kinetics as well as with one-step global kinetics" (Bowen, Holmes, et al. 1999, p. 19).

Research success depends on the team's considerable experience combined with recently published studies on comprehensive modeling of hydrocarbon oxidation, which employ detailed chemical kinetics. Dr. Gogos' doctoral student, Daniel Pope, is supported under the NASA Nebraska Space Grant and EPSCoR Programs. He has been working for over two years simulating combustion of a moving droplet with one-step kinetics and contributes immensely to the timely completion of the proposed work.

Additionally, data obtained from NASA sponsored studies are available in current literature and additional data will soon become available. This model will be compared and validated against these experimental data. The UNO CEFD team "expects to capture the nonlinear interaction between hydrodynamics and detailed chemical kinetics, which will lead to an extremely valuable appropriately-validated model for combustion of a moving fuel droplet" (Bowen, Holmes, et al., 1999, p. 19).

Research Progress

The current CEFD CRT research has focused on the development of a validated

numerical model for droplet combustion in a forced convection environment. Funded by the

previous five-year NASA EPSCoR grant, a quasi-steady numerical model, which utilized one-

step overall chemical kinetics and a single diffusion coefficient to describe the mass diffusion,

was developed to study the convective extinction of fuel droplets under zero-gravity conditions

(Gogos, Pope, & Lu, 2001, p. 2). As a result of suggestions made in the review of the 2001 Pope

and Gogos article and as a prelude to incorporating multi-step chemical kinetics schemes, the

quasi-steady code is currently being modified to allow for the different mass diffusion

coefficients associated with each pair of chemical species. This modification to the quasi-steady

code is part of the systematic addition of modeling complexities that was presented in the

original research proposal. The end goal of the research is to develop an experimentally

validated droplet combustion model that can be used for accurate predictions of single droplet

behavior in practical combustion systems.

The conditions present in convective droplet combustion experiments are different from

those present in practical combustion systems. Droplet combustion experiments under forced

convection are conducted by suspending the fuel droplet from a silica fiber in an ambient

oxidizer at a fixed temperature ($T\infty$) and pressure ($p\infty$), as shown in Figure 1. The oxidizer is

"blown" over the droplet at some fixed velocity ($U\infty$). If the ambient temperature is high

enough, or if an external ignition source is present, the droplet will ignite. The initial flame

configuration (wake, transition, or envelope) depends on the "blowing" velocity. In practical

combustion systems, droplets are injected into a combustion chamber. This situation is shown in

Figure 2, where the droplet is injected, at some initial velocity, into a stagnant environment at a

specified temperature and pressure. The moving droplet experiences a drag force that opposes its motion and the droplet velocity decreases. The initial velocity determines the initial flame configuration. If the initial flame configuration is a wake flame, the decrease in droplet velocity can result in a change from a wake to a transition flame, and finally to an envelope flame. The numerical model must be able to deal with both the suspended droplet case (for model validation) and the moving droplet case (for practical predictions). A transient code is required to model the change in droplet diameter caused by evaporation at the droplet surface, the change in flame position and configuration, the internal heating of the droplet, and the decrease in droplet velocity for the moving droplet.

A transient code has been developed to model droplet combustion in a forced convection, zero-gravity environment. One-step overall chemical kinetics and a single diffusion coefficient to describe the mass diffusion were used in the model. The model has been validated using the numerical results of the 2001 Gogos and Zhang research for the evaporation (no combustion) of n-heptane droplets in nitrogen at atmospheric pressure. Excellent quantitative agreement was observed for various ambient temperatures and initial droplet velocities.

The transient code has been used to numerically investigate the combustion of n-heptane droplets in air at atmospheric pressure. The initial droplet diameter (D0 = 0.5mm), initial droplet temperature (T0 = 297K), and the ambient temperature (T∞ = 1000K) were fixed and the initial droplet velocity (U∞(0)) or "blowing" velocity (U∞) was varied. Results have been obtained for moving and suspended droplets with initial Reynolds numbers of 10, 25, 50, and 100. At a given initial Reynolds number, the fixed "blowing" velocity (suspended droplet) and the initial droplet velocity (moving droplet) are equal. The numerical results indicate that the initial Reynolds number determines the flame configuration that forms during droplet ignition for both moving

and suspended droplets. An envelope flame is formed during droplet ignition for an initial Reynolds number of 10 and a wake flame is observed at the higher initial Reynolds numbers. This is in qualitative agreement with the quasi-steady code, which predicts an envelope flame for Reynolds numbers less than 12 under these same conditions. Once the initial flame configuration had formed (either envelope or wake), the suspended droplet cases exhibited the same flame configuration throughout the droplet lifetime. In the moving droplet cases, the wake flame that formed at the higher initial Reynolds numbers, gradually approached, and then eventually surrounded the droplet in an envelope flame configuration as the droplet velocity decreased. The predictions indicate a marked difference between the behavior of suspended and moving droplets.

The development of a transient droplet combustion code represents a significant step in our current research which is funded by the new five-year NASA EPSCoR grant. The modification of the quasi-steady code to include multiple diffusion coefficients is nearing completion. Once this modification is tested, it will be incorporated in the transient model. The next step will then involve the incorporation of multi-step chemical kinetics in the quasi-steady and transient models.

Research Outcomes

The CEFD CRT meets weekly to provide an opportunity for researchers to present and discuss their new results. This ensures that research objectives are being met. For additional dissemination of findings, this CRT established collaboration with both the John Glenn Research Center at Lewis Field in Ohio and the U.S. Department of Defense. Continued communication is also a priority for the CEFD team. Additionally, Principal Investigator Gogos' has maintained direct communication with Dr. Vedha Nayagam in San Diego, California. This communication

will allow the CEFD CRT's modified numerical code to be validated by Dr. Nayagam's experimental data.

A post doctorate research associate, Dr. Daniel Pope, and a research assistant professor, Dr. Hongtao Zhang, are also participants in this research project. Both researchers have set goals of becoming tenure track faculty in institutions of higher education. The weekly research meetings provide both Dr. Pope and Dr. Zhang with invaluable experience on graduate student advising. Additionally, they are strongly involved in every other aspect of the CEFD research faculty such as, writing proposals, writing papers, presenting conference papers, reviewing papers. Such mentoring opportunities are expected to continue throughout the lifetime of the research study.

Conclusion

The Numerical Simulation of the Combustion of Fuel Droplets study is one of three Collaborative Research Teams (CRT) currently supported by the NSGC & EPSCoR programs. Each CRT strives to provide the most current information to interested members of the academic world. The Numerical Simulation of the Combustion of Fuel Droplets study is an evolving project. Periodic updates are available on a quarterly basis.

Additional collaborations are sought with other organizations on a continual basis. All opportunities for collaboration are invited for consideration. Additionally, NSGC & EPSCoR welcome any input on program directions as well. The partnership between the NSGC & EPSCoR programs allows for the selection of outstanding research projects that positively impact aeronautical technology advancement. Those in the NSGC & EPSCoR program, the Collaborative Research Teams, and the industry look forward to experiencing the same high level of achievement in the future.

Further Information

If you would like further information regarding the Numerical Simulation of the

Combustion of Fuel Droplets, or would like to collaborate with the Nebraska CRT, please

contact:

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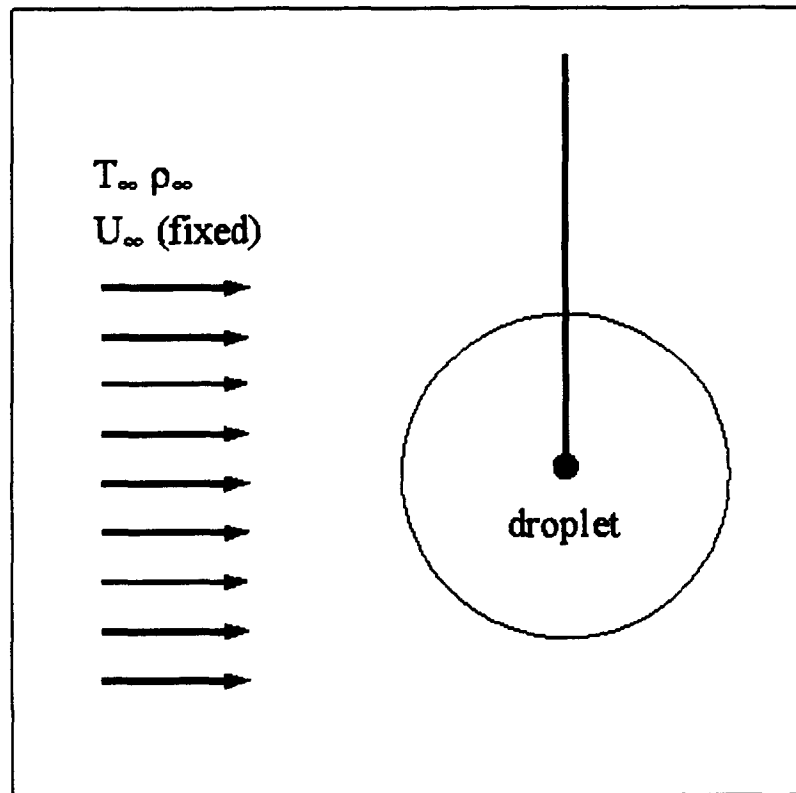TEL: 402/554-3772; FAX 402/554-3781

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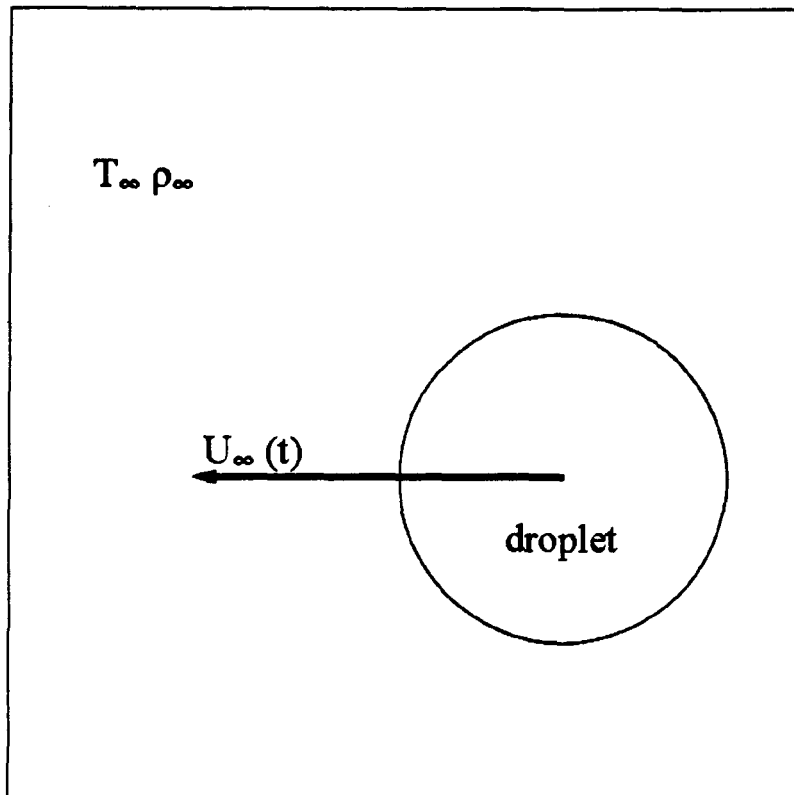
Figure Caption

Figure 1. Orientation of single droplets for experiments

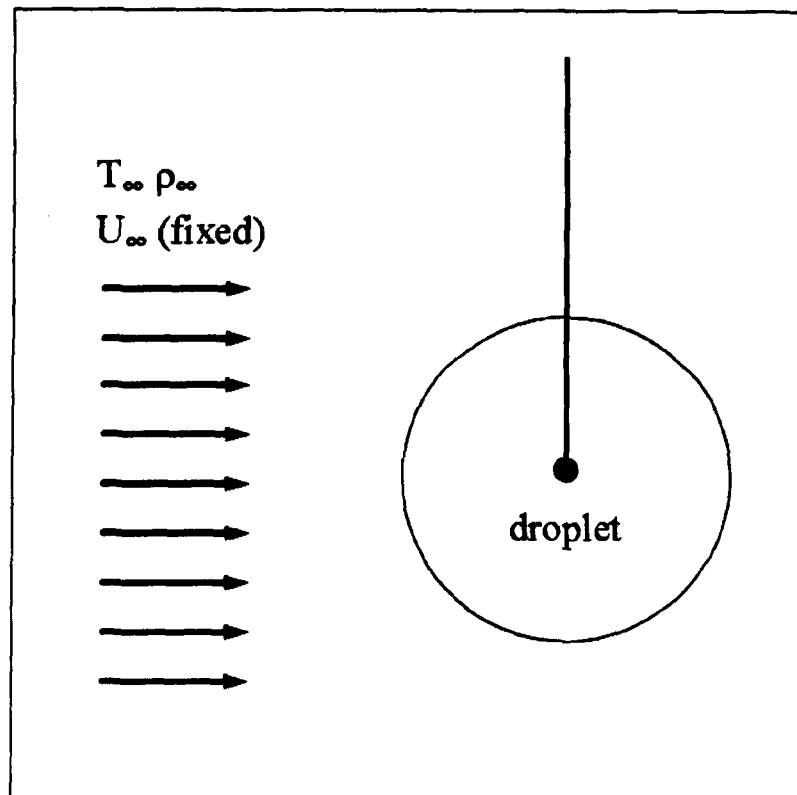Figure 2. Orientation of single droplets within practical combustion systems.

This overview was prepared by Mrs. Jocelyn Nickerson, Dr. Brent Bowen, Dr. George Gogos

and various CEFD CRT members. Last update occurred on June 4, 2002 at 2:58 PM.

T_∞ ρ_∞
U_∞ (fixed)

droplet

Suspended Droplet

Moving Droplet

T_∞ ρ_∞
U_∞ (fixed)

droplet

Suspended Droplet